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Title: PHYSICS MODELS AND NUCLEAR DATA EVALUATIONS FOR ENHANCED MONTE-CARLO TRANSPORT

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Physics models and nuclear data evaluations for enhanced Monte-Carlo transport

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Abstract. We describe recent evaluations of neutron and proton interaction cross sections up to 150 MeV in the LA150 Data Library, for use in MCNPX computer code simulations of accelerator-driven systems (ADS). An overview is provided of the nuclear theory used. A number of benchmark comparisons against experiments are described, for thin and thick-target neutron production, neutron transmission through macroscopic slabs, and neutron heating and damage. Future data needs for waste transmutation are also briefly described.

1 Model calculations for the LA150 databases

A suite of evaluated reaction cross section files collectively known as the LA150 Library has been developed [1,2] in support of accelerator-driven systems design. These evaluations are in ENDF-6 format, and have recently been accepted into the U.S.-standard ENDF/B-VI Library as Release-6. For incident neutrons, they extend the previously-existing ENDF/B-VI information from 20 MeV up to 150 MeV. For incident protons, the files extend from 1–150 MeV. To date, evaluations have been completed for isotopes of the following structural, shielding, and target-blanket materials: H, Li, C, N, O, Al, Si, P, Ca, Fe, Ni, Cr, Cu, Nb, W, Hg, Pb, and Bi.

These LA150 evaluated cross sections are designed for use in radiation transport codes, such as the MCNPX code [3]. The primary motivation for using these evaluated data is the accuracy improvements that one can expect to obtain in the below-150 MeV energy region. In most previous transport simulations, intranuclear-cascade methods have been used for neutrons above 20 MeV and for protons at all energies, even though the semiclassical assumptions inherent within such models do not hold at lower energies. By developing evaluated cross section libraries up to 150 MeV, using state-of-the-art nuclear reaction models in the GNASH code as well as experimental data, one can expect to have the most accurate possible representation of the nuclear cross sections.

The nuclear models used are based on theoretical approaches that are appropriate for the energies in the few-MeV to 150 MeV range: the Hauser-Feshbach compound nucleus theory; preequilibrium calculations based on the Feshbach-Kerman-Koonin theory or the exciton model; direct reactions calculated from the optical model using collective excitation form factors; and elastic scattering from the optical model. The GNASH code was demonstrated to be one of the most accurate codes available for model calculations below 150 MeV in a Nuclear Energy Agency code intercomparison [4].

The optical model is used for predictions of the total, reaction, and elastic scattering cross sections, making use of nucleon potentials at higher energies developed by Madland [5], Chiba, and Koning. It is particularly useful for accurately representing the angular distributions in elastic scattering, allowing more accurate neutron transport simulations. (Many previous intranuclear cascade transport codes instead represent elastic scattering using a black-disc diffraction formula or use even simpler approaches, which poorly approximate reality below a few hundred MeV.)

2 Results

2.1 Neutron multiplication in (n, xn) and (p, xn) reactions

Neutron multiplication reactions play an important role in spallation targets, and when the nucleon energies fall below 150 MeV much of the neutron production comes from (n, xn) rather than (p, xn) reactions. This is simply because the probability that protons below 150 MeV stop before having a nuclear reaction is significant. Because of this, we have placed a large emphasis on accurately modeling the (n, xn) reactions.

An example is shown in Fig. 1 (left-hand-side) for the 26 MeV ^{209}Bi(n, xn) angle-integrated secondary neutron spectrum, where measurements exist [6]. The figure shows the components of the calculated spectrum due to compound nucleus emission, preequilibrium emission, and direct reactions. The direct reactions were calculated using Distorted-Wave Born Approximation theory. Collective excitations of excited vibrational states were treated using the weak-coupling model, with a $h_{9/2}$ proton coupled to a ^{208}Pb core. This allows extensive deformation-length information from direct reactions on ^{208}Pb to be used in the bismuth calculations.

Figure 1 (right-hand-side) shows the calculated 113 MeV Pb(p, xn) neutron energy spectra at various angles, compared with data [7]. Agreement is good except at the backward angle where the calculations underpredict the experiment in the preequilibrium region. At low energies the large evaporation peak from sequentially-emitted compound nucleus neutrons is evident. Above about 10 MeV, the spectra have a hard preequilibrium tail that extends up to the incident energy minus the Q-value. These preequilibrium neutrons are seen to be strongly forward-peaked, whereas the evaporation neutrons are approximately isotropic.

2.2 Proton-induced thick-target neutron production

It is important for nuclear simulation codes to adequately predict secondary neutron production from protons as they traverse target, blanket, and shielding materials. Secondary neutron production is central to spallation neutron target design, beam-stop design, and shielding considerations. Thick-target neutron

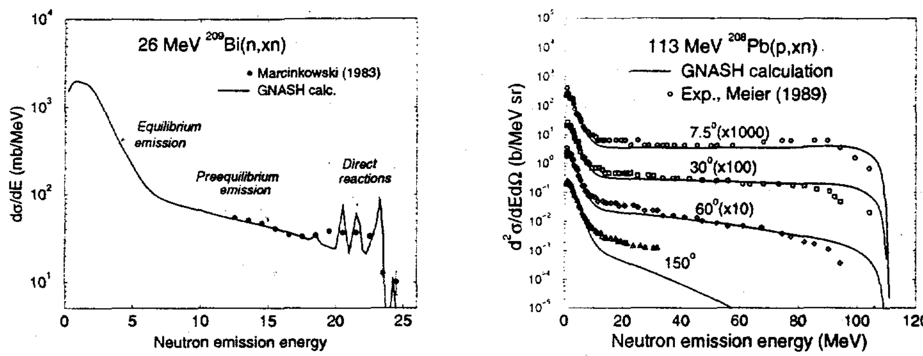

Fig. 1. (a) *l.h.s.:* Measured secondary angle-integrated neutron spectrum for 26 MeV neutrons on bismuth compared with GNASH calculations used in the LA150 Library; (b) *r.h.s.:* Evaluated ^{208}Pb(p, xn) double-differential neutron emission spectra compared with experimental data [7] at 113 MeV incident energy.

production measurements provide an ideal way to test the microscopic nuclear data, in this case the LA150 proton data library, and test the proton transport algorithms used within MCNPX. Such measurements are usually made for targets that are sufficiently thick to stop the incident protons, though the targets are generally "thin" as far as the secondary neutrons are concerned. Thus, the probability that a secondary neutron produced has a subsequent nuclear interaction within the target is small. The protons slow down from their maximum energy, and for the maximum energy and all lower energies they have a probability of undergoing nuclear collisions leading to neutron production. Thick-target measurements therefore represent an integral over all incident energies up to the maximum of the differential "thin-target" cross sections, weighted by the stopping power function.

At 68 MeV and 113 MeV, proton-induced thick-target neutron production has been measured [7,8]. These data are compared with our MCNPX calculations in Fig. 2. The MCNPX with LA150 data simulation appears to more accurately describe the emitted neutron spectra compared to use of LAHET physics.

2.3 Neutron transmission and shielding design

Japanese measurements [9] have been particularly useful for assessing the capabilities of a simulation code for shielding studies. A quasi-monoenergetic neutron source was generated by bombarding a Li target with 68 MeV protons, using the Li(p,n) reaction. These neutrons subsequently impinged upon macroscopic slabs of iron and concrete, of various thicknesses. The transmitted neutrons were then measured at locations both on and off the beam's axis. We demonstrated [1] that, compared to LAHET simulations, significant gains can be obtained when modeling neutron transmission through iron by use of the LA150 data in

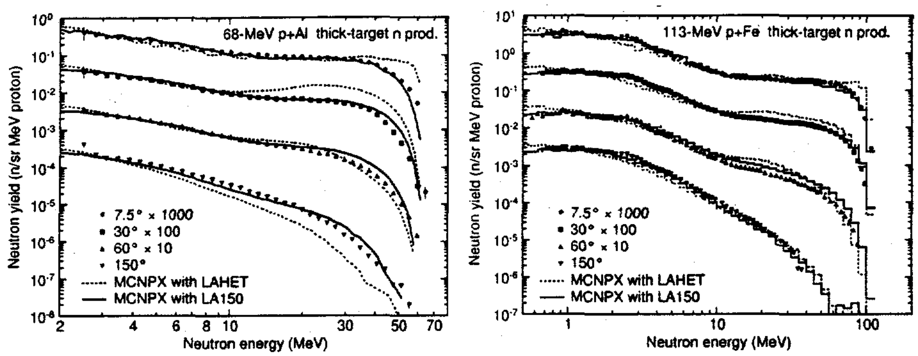

Fig. 2. Thick target neutron production spectra for: (a) *l.h.s.*: 68 MeV protons incident on aluminum [8] compared with calculations; (b) *r.h.s.*: 113 MeV protons incident on iron [7]. The solid lines show MCNPX using the LA150 data, the dashed lines show MCNPX using LAHET physics.

MCNPX. Similar conclusions were also obtained by Sweezy *et al.* [10] who used MCNPX with LA150 data to simulate broad-spectrum neutron transmission through shields of iron, lead, concrete, and graphite.

2.4 Radiation heating and damage

The LA150 cross section data were developed with an emphasis on providing an accurate description of energy deposition, for radiation heating calculations. One of the reasons for this was their use in medical applications for calculations of absorbed dose in fast neutron and proton radiotherapy [11,12]. Radiation heating is also important in accelerator-driven systems. Comparisons between our evaluated neutron kerma coefficients and measured values are given in Refs. [11,12].

The NJOY Nuclear Data Processing System has, since 1979, been capable of calculating the neutron damage energy cross section. A description of the theory of damage energy and the computation of damage energy are described in the NJOY Manual, Chapter 4 [13]. This cross section is used to calculate lattice defect production rates in materials, which are an important measure of radiation damage. The LA150 Library is the first Los Alamos release of a continuous-energy MCNPX library to include the damage energy cross section. For accelerator applications, this cross section is a welcomed addition as radiation damage effects are particularly severe in accelerator-driven neutron sources.

At energies above nuclear data evaluations, the LAHET code [14] may be used to generate the damage energy cross section. The LAHET code relies on physics models of the intranuclear cascade in calculating the damage energy cross section, and again these are known to be less reliable at energies below approximately 150 MeV. The community that uses damage energy cross section data has noted a substantial discrepancy between evaluated damage energy cross

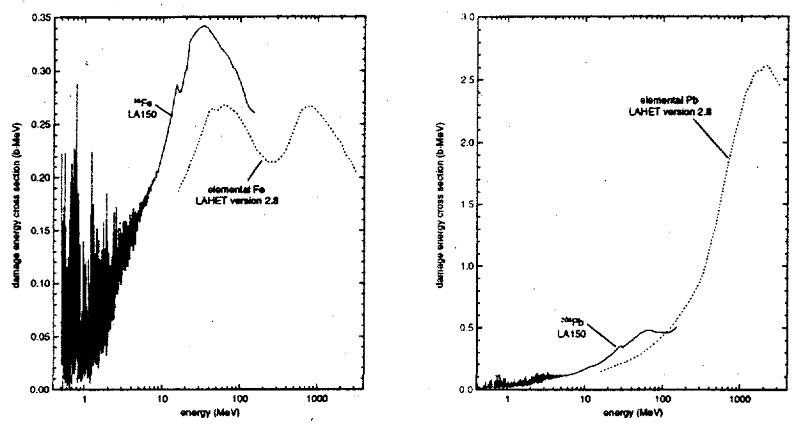

Fig. 3. The neutron damage energy cross section [13] from the LA150 Library over the energy range 400 keV to 150 MeV for ^{56}Fe and ^{208}Pb. Also plotted is the damage energy cross section as calculated using LAHET version 2.8 over the energy range 16 MeV to 3.1 GeV.

sections and those generated by LAHET at the traditional transition energy of 20 MeV. The extension of this transition energy to 150 MeV brought about by the advent of the LA150 Library reduces the observed discrepancy. In figure 3 we plot the damage energy cross section from the LA150 Library over the energy range 400 keV to 150 MeV for ^{56}Fe and ^{208}Pb. Also plotted is the damage energy cross section as calculated using LAHET version 2.8 over the energy range 16 MeV to 3.1 GeV for the elements corresponding to the isotopes [15]. For the representative isotopes considered here, the agreement between the evaluated data and the LAHET-generated data is generally better at 150 MeV than at 20 MeV. This is consistent with expectations since LAHET should be less reliable at the lower energy.

3 Future Work and ATW

In order to build upon the work described here for use in the accelerator-transmutation of waste (ATW) program, a number of advances will be needed. First and foremost is a focus on nuclear cross section data for minor actinides and fission products, as well as for nuclides used in the spallation target and coolant (e.g. Bi, Pb, and possibly W or depleted U). Although some higher energy particles from the spallation target will enter the transmuter (subcritical reactor), the main focus for the transmuter will be on cross section data below

20 MeV at fast neutron energies. We anticipate that experimental work will also be needed to guide the calculations and evaluations, particularly for fission and capture processes.

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